

Generalizations of Kijowski's time-of-arrival distribution for interaction potentials

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Several proposals for a time-of-arrival distribution of ensembles of independent quantum particles subject to an external interaction potential are compared making use of the “crossing state” concept. It is shown that only one of them has the properties expected for a classical distribution in the classical limit. The comparison is illustrated numerically with a collision of a Gaussian wave packet with an opaque square barrier.

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I. INTRODUCTION

In many experiments, the observed quantities are the instants of occurrence of certain events, or the durations of processes. However, the standard quantum formalism does not provide, at least in an obvious manner, a working rule for time observables. In spite of the difficulties and objections to consider time as a quantum observable (by Pauli [1], Allcock [2], and other authors), many researchers have sporadically tried to fill this theoretical lacuna. The effort in that direction has become more intense and systematic in recent years. In particular, much attention has been devoted to the quantum description of the “arrival time” [3–27], see [24] for a recent review. In its simplest form, the problem is to define an ideal quantum arrival time distribution for a wave packet moving freely in one dimension. By imposing a number of classically motivated conditions (normalization, positivity, minimum variance, and a certain symmetry with respect to the arrival point X) this is solved uniquely by Kijowski's distribution [3]. This distribution may also be associated with the positive operator valued measure (POVM) generated by the improper eigenstates of the time-of-arrival maximally symmetric operator of Aharonov and Bohm [28], \hat{T}_{AB} ,

$$\hat{T}_{AB} = \frac{mX}{\hat{p}} - \frac{m}{2} \left(\hat{x} \frac{1}{\hat{p}} + \frac{1}{\hat{p}} \hat{x} \right), \quad (1)$$

where \hat{x} and \hat{p} are position and momentum operators and m is the mass. Aside from the discussion of remaining interpretational puzzles, an important pending question is its generalization for particles affected by interaction potentials [24]. However, Kijowski's set of conditions cannot be applied in the general case [3], where, classically, not all particles necessarily arrive, or multiple arrivals may have to be considered. Neither can the simple symmetrization rule leading to \hat{T}_{AB} be used [29]. Thus a generalization of Π_K required some novel approach and it is only very recently that some of them have been explored, following different heuristic and/or formal arguments. Their physical content must be analyzed in order to select one that does fit into the proposed objective (although several might be adequate). This is the aim of the present paper, where we shall examine three possible generalizations of Kijowski's distribution. The unifying framework is provided by the concept of “crossing state” introduced in [23], and inspired by Wigner's formalization of the time-energy uncertainty principle [30]. In all the proposals examined here the (candidate) time-of-arrival distribution at point X may be obtained from the overlap of the time dependent wave function and the crossing states $|u^\beta(X)\rangle$ as

$$\Pi(T) = \sum_{\beta} \Pi^\beta(T) = \sum_{\beta} |\langle \psi(T) | u^\beta(X) \rangle|^2, \quad (2)$$

where $\beta = L, R$ is an index for “left” and “right”; its exact meaning will vary in the different generalizations. We shall use a unified notation that will differ in general from that of the original papers to facilitate the common presentation and comparison. Incidentally, all distributions defined in this manner are automatically covariant with respect to time translations, namely, the arrivals predicted for a given fixed instant are independent of the choice made for the origin of time [25,24].

II. DIFFERENT CROSSING STATES

A. Free motion

Kijowski's distribution is obtained from the general expression (2) with the following crossing states (their coordinate representation, time evolution, and wave packets peaked around them have been studied in [10]),

$$|u^\beta(X)\rangle_K = (|\hat{p}|/m)^{1/2} \Theta(\alpha \hat{p}) |X\rangle, \quad (3)$$

where

$$\alpha = \begin{cases} + & \text{if } \beta = L \\ - & \text{if } \beta = R, \end{cases} \quad (4)$$

$|\hat{p}|^{1/2}$ is defined by its action on plane waves,

$$|\hat{p}|^{1/2} |p\rangle = |p|^{1/2} |p\rangle, \quad (5)$$

(the positive root is taken), and Θ is the Heaviside distribution.

Now we can write Kijowski's distribution in operator form as

$$\Pi_K(T) = \sum_{\alpha} \langle \psi(T) | \left[\Theta(\alpha \hat{p}) (|\hat{p}|/m)^{1/2} \delta(X - \hat{x}) (|\hat{p}|/m)^{1/2} \Theta(\alpha \hat{p}) \right] | \psi(T) \rangle. \quad (6)$$

Each of the operators in brackets (with $\alpha = +$ or $-$ respectively) corresponds classically, i.e., disregarding the lack of commutativity between \hat{x} and \hat{p} , to the classical dynamical variable

$$\delta(x - X) \frac{\alpha p}{m} \Theta(\alpha p), \quad (7)$$

whose average $\langle \dots \rangle_{cl}$ over a classical phase space density gives the flux due to particles arriving from the left, J_{cl}^L , or minus the flux due to particles arriving from the right, $-J_{cl}^R$ (which is a positive quantity, $-J_{cl}^R > 0$),

$$\alpha J_{cl}^\beta = \langle \delta(x - X) \frac{\alpha p}{m} \Theta(\alpha p) \rangle_{cl}, \quad (8)$$

in other words, the modulus of the flux of particles of the classical ensemble that arrive from one side at a given time [8]. The addition of these two contributions is the classical time-of-arrival distribution,

$$\Pi_{cl}(T) = J_{cl}^L - J_{cl}^R \quad (9)$$

B. Interacting case: first proposal

The previous discussion motivates the first generalization of Π_K considered here for independent particles affected by an arbitrary interaction potential. Since (9) is valid regardless of the presence of a potential, and the dynamical variables for the two flux contributions are always given by (7), it was proposed in [23] that the quantum time-of-arrival distribution in the general case be given by the same expression used in the free motion case, Eq. (6), and by the same crossing states, $|u^\beta\rangle_1 = |u^\beta\rangle_K$, as they lead to operators in correspondence with the classical expression (7). In other words, the proposed distribution is given by

$$\Pi_1(T) = \sum_{\beta} |\langle \psi(T) | u^\beta \rangle_K|^2, \quad (10)$$

where now ψ evolves with the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ which includes a kinetic term, \hat{H}_0 , and a potential term, \hat{V} . We are thus extending to the quantum domain the fact that in classical mechanics the expressions for dynamical variables representing the partial fluxes do not vary from the free-motion case to the interacting case. Here, the state $(\psi(T)$ quantally, and the evolved phase space density classically), rather than the dynamical variable, contains the information which is specific to each particular Hamiltonian. At the very least, this generalization of Kijowski's distribution has the merit of being simple, arguably the simplest one. Further properties were commented in the original paper [23]. In particular, note that (10) need not be normalized, and in fact may be not normalizable, as may also be the case classically, e.g. because of periodic crossings in a harmonic potential. It can also be defined even if the system is not classically integrable.

C. Interacting case: second proposal

The other two definitions discussed here are applicable to “scattering potentials” where Möller operators exist,

$$\hat{\Omega}_{\pm} = \lim_{t \rightarrow \mp\infty} e^{i\hat{H}t/\hbar} e^{-i\hat{H}_0 t/\hbar}. \quad (11)$$

We shall assume that the potential operator \hat{V} has a local coordinate representation

$$\langle x|\hat{V}|x'\rangle = \delta(x - x')V(x), \quad (12)$$

with potential function $V(x)$ vanishing at long distances from the interaction region so that the (strong) limits in Eq. (11) exist. As usual, we shall also consider, with the same notation, extensions of these Hilbert space operators that can be applied to plane waves,

$$|p_{\pm}\rangle = \hat{\Omega}_{\pm}|p\rangle \equiv |p\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_p \pm i\varepsilon - \hat{H}} \hat{V}|p\rangle, \quad E_p = p^2/2m. \quad (13)$$

The Lippmann-Schwinger states $|p_{\pm}\rangle$ are improper (not square integrable) eigenstates of \hat{H} with eigenvalue E_p . $\hat{\Omega}_{\pm}$ are in general only isometric, i.e., they conserve norm, but in the absence of bound states they become also unitary. We shall limit ourselves to this later case hereafter. The physical meaning of $\hat{\Omega}_{\pm}$ is best understood with the aid of “asymptotic” incoming and outgoing states, ϕ_{in} and ϕ_{out} , to which the actual state ψ tends in a strong sense in the infinite past and future, respectively. These asymptotic states evolve freely, with \hat{H}_0 . Whereas $\hat{\Omega}_+$ provides the scattering state by acting on the incoming asymptote, $\hat{\Omega}_-$ does the same job acting on the outgoing one,

$$\hat{\Omega}_+|\phi_{in}(t)\rangle = |\psi(t)\rangle, \quad (14)$$

$$\hat{\Omega}_-|\phi_{out}(t)\rangle = |\psi(t)\rangle, \quad (15)$$

for all t .

Without bound states, the resolution of unity can be written equivalently as

$$\hat{1} = \int_{-\infty}^{\infty} dp |p\rangle\langle p| = \int_{-\infty}^{\infty} dp |p_{\pm}\rangle\langle p_{\pm}|, \quad (16)$$

and the Hamiltonians \hat{H}_0 and \hat{H} may be related by the unitary transformation

$$\hat{H} = \hat{\Omega}_{\pm}\hat{H}_0\hat{\Omega}_{\pm}^{\dagger}, \quad (17)$$

with a similar relation holding for functions of \hat{H}_0 and \hat{H} . This suggests using the crossing states

$$|u_{\pm}^{\beta}(X)\rangle_2 = \hat{\Omega}_{\pm}|u^{\beta}(X)\rangle_K. \quad (18)$$

Note the additional subscript in the crossing state, + or −, due to the possibility to act with either one of the two Möller operators on $|u^{\beta}\rangle_K$. Thus, this procedure generates two different distributions labelled by + or −,

$$\Pi_{2,\pm} = \sum_{\beta} |\langle\psi(T)|u_{\pm}^{\beta}(X)\rangle_2|^2. \quad (19)$$

These distributions previously appeared in [20] (later superseded by [21]). It is important to notice that this is not the way in which the original distributions in [20] were presented; they have been adapted here to the unified notation we are using in order to achieve a better handle for comparison. Their physical content is made evident by making use of (14), (15), and the isometry of the Möller operators,

$$\langle\psi(T)|\hat{\Omega}_+|u^{\beta}(X)\rangle_K = \langle\phi_{in}(T)|\hat{\Omega}_+^{\dagger}\hat{\Omega}_+|u^{\beta}(X)\rangle_K = \langle\phi_{in}(T)|u^{\beta}(X)\rangle_K, \quad (20)$$

$$\langle\psi(T)|\hat{\Omega}_-|u^{\beta}(X)\rangle_K = \langle\phi_{out}(T)|\hat{\Omega}_-^{\dagger}\hat{\Omega}_-|u^{\beta}(X)\rangle_K = \langle\phi_{out}(T)|u^{\beta}(X)\rangle_K. \quad (21)$$

This means that the generated distributions, $\Pi_{2,+}$ and $\Pi_{2,-}$ are nothing but the Kijowski distributions corresponding to the incoming and outgoing free-motion asymptotes, respectively. These may be useful objects before ($\Pi_{2,+}$) and after ($\Pi_{2,-}$) the collision, but not in the midst of it.

D. Interacting case: Third proposal

A different, more complex proposal is based on the following crossing states,

$$|u_{\pm}^{\beta}(X)\rangle_3 = \hat{\Omega}_{\pm} \Theta(\alpha \hat{p}) (|\hat{p}|/m)^{1/2} \hat{\Omega}_{\pm}^{\dagger} |X\rangle, \quad (22)$$

which lead again to two different distributions,

$$\Pi_{3,\pm}(T) = \sum_{\beta} |\langle \psi(T) | u_{\pm}^{\beta}(X) \rangle_3|^2. \quad (23)$$

These distributions were first introduced and discussed by León et al. in [21], as justified by quantization through quantum canonical transformations of the classical time of arrival (see also [22] for further analysis of this proposal). As previously stated, the rewriting in terms of crossing states is intended to clarify the physical consequences of these distributions. To analyze their meaning, let us first study the amplitudes corresponding to $\hat{\Omega}_{+}$, by inserting $\hat{1} = \hat{\Omega}_{+}^{\dagger} \hat{\Omega}_{+}$, and rewriting them as

$$\langle \psi(T) | \left[\hat{\Omega}_{+} \Theta(\alpha \hat{p}) \hat{\Omega}_{+}^{\dagger} \right] \left[\hat{\Omega}_{+} (|\hat{p}|/m)^{1/2} \hat{\Omega}_{+}^{\dagger} \right] |X\rangle. \quad (24)$$

The operators involved have been separated in two brackets that can be interpreted physically. The first one is a projector that selects the part of a wave function that *had* positive ($\alpha = +$) or negative momentum ($\alpha = -$) in the infinite past,

$$\hat{F}_{+}^{\beta} \equiv \hat{\Omega}_{+} \Theta(\alpha \hat{p}) \hat{\Omega}_{+}^{\dagger} = \alpha \int_0^{\alpha\infty} dp |p_{+}\rangle \langle p_{+}|; \quad (25)$$

the second group of operators is

$$(2\hat{H}/m)^{1/4} \equiv m^{-1/2} \hat{\Omega}_{+} |\hat{p}|^{1/2} \hat{\Omega}_{+}^{\dagger} = \int_{-\infty}^{\infty} dp |p_{+}\rangle (2E_p/m)^{1/4} \langle p_{+}|, \quad (26)$$

where the positive root is taken. For the case in which the incoming asymptote is restricted to positive momenta,

$$\langle \psi(T) | \hat{F}_{+}^L = \langle \psi(T) |, \quad (27)$$

$$\langle \psi(T) | \hat{F}_{+}^R = 0, \quad (28)$$

so that the proposed distribution takes the form

$$\Pi_{3,+}(T) = \Pi_3^L(T) = \langle \psi(T) | (2\hat{H}/m)^{1/4} \delta(\hat{x} - X) (2\hat{H}/m)^{1/4} | \psi(T) \rangle. \quad (29)$$

The resulting operator is a quantum symmetrization of the classical phase space dynamical variable

$$(2E/m)^{1/2} \delta(x - X), \quad (30)$$

E being the *total* energy, to be compared with the classical variables of the first generalization which lead to the positive and minus negative fluxes,

$$(|p|/m) \Theta(p) \delta(x - X), \quad (31)$$

$$(|p|/m) \Theta(-p) \delta(x - X). \quad (32)$$

Note that, for an X such that $V(X) = 0$, the (classical) average of (30) is equal to the average of the sum of (31) and (32), i.e. to the time of arrival distribution,

$$\langle (2E/m)^{1/2} \delta(x - X) \rangle_{cl} = J_{cl}^L - J_{cl}^R, \quad \text{if } V(X) = 0. \quad (33)$$

However, in the interaction region, it is in fact proportional to the local square root of the total energy. This may lead to significant differences with the actual time-of-arrival distribution, which classically is always given by $J_{cl}^L - J_{cl}^R$ irrespective of the value of $V(X)$. In particular, for a potential barrier such that the initial (asymptotic) momenta of the particles slow down on its top to a smaller value, (30) will overestimate the value of the true arrival time

distribution, since for each trajectory the square root $(2mE)^{1/2}$ is used, instead of the smaller local momentum that determines the partial fluxes. Note also that the superscript L in (29) does not make reference here to actual crossing from the left in the classical limit, but to motion from the left *in the infinite past*. In this respect, (30) equally counts right or left crossings at a given time.

A similar analysis may be carried out for a state with incoming asymptote in the subspace of negative momenta. Thus, for an arbitrary initial state with positive and negative momentum components, $\Pi_{3,+} = \Pi_{3,+}^L + \Pi_{3,+}^R$ provides a quantum version of the distribution that corresponds to the classical dynamical variable (30). Repeating the same steps with $\hat{\Omega}_-$, $\Pi_{3,-}^\beta$ may be interpreted as the quantum versions of the classical distributions of (30) for particles that will have positive or negative momenta in the infinite future.

III. NUMERICAL EXAMPLE

We shall illustrate the results of the previous section with the collision of a wave packet for a particle of mass $m = 1$ with a square barrier. The initial state (at $t = 0$) is chosen as a minimum-uncertainty-product Gaussian with negligible negative momentum components. Its average position, average momentum, and standard deviation are for the first four figures, in atomic units,

$$\langle \hat{x} \rangle = -6, \quad \langle \hat{p} \rangle = 6, \quad \Delta x = 1, \quad (34)$$

whereas the barrier energy, initial and final points are

$$V_0 = 10, \quad x_i = 0, \quad x_f = 10. \quad (35)$$

With these parameters the barrier is rather opaque. This prevents tunneling and makes the collision predominantly classical. The figures combine variously the different distributions, their components, and the flux for the three points, $X = -2, 5, 12$, corresponding to positions before, in, and after the barrier respectively. The evaluation of the integrals requires explicit representations of the states $|p_\pm\rangle$ that can be found elsewhere [31].

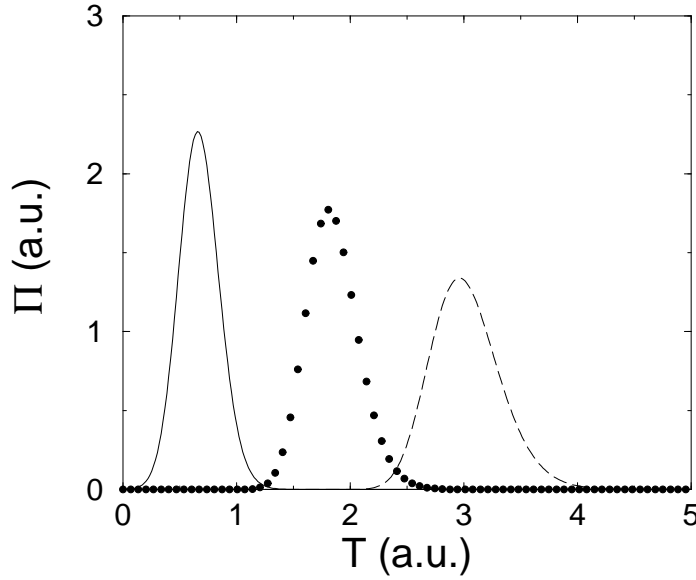


FIG. 1. Π_K and $\Pi_{2,+}$ (which overlap) for $X = -2, 5$ and 12 (solid, dotted, and dashed lines) for the Gaussian wave packet described in the text, see (34).

Fig. 1 represents Kijowski's distribution for the case in which the wave packet evolves freely, without interaction with the barrier, as well as $\Pi_{2,+}$ in the interacting case. Since the fraction of negative momenta in the initial state is negligible, it may be considered essentially equal to the corresponding incoming asymptotic state for the numerical accuracy of the figures. Thus $\Pi_{2,+}$ (or $\Pi_{2,+}^L$) and Π_K are indistinguishable for the three values of X .

Fig. 2 shows $\Pi_{2,-}^L$ and the flux J , before, in, and after the barrier, which is now present. They coincide after the barrier, for $X = 12$, but differ otherwise. This is to be expected since $\Pi_{2,-}^L$ is a free-motion Kijowski distribution for the positive momentum part of the outgoing asymptotic state.

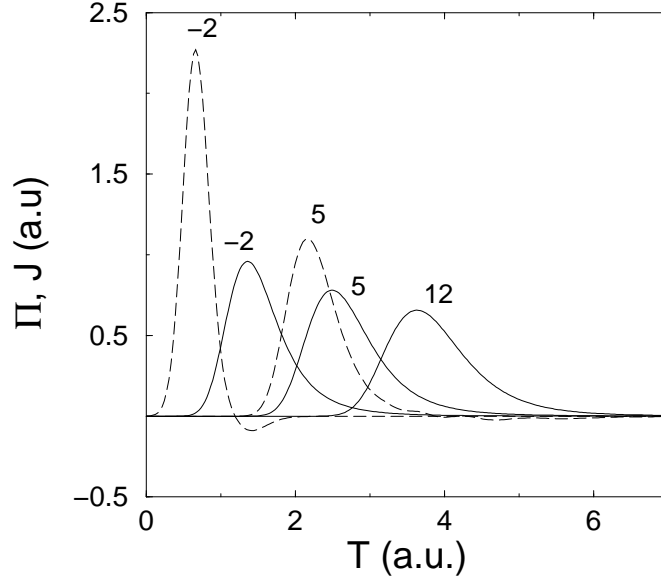


FIG. 2. $\Pi_{2,-}^L$ and J (solid and dashed lines respectively) for $X = -2, 5$ and 12 (indistinguishable in the later case).

At $X = -2$, where the potential vanishes, Π_1 and $\Pi_{3,+}$ are in essential agreement, see Fig. 3. The second, smaller bump corresponds to the period of negative flux due to a small reflection. This smaller bump is due to a contribution of Π_1^R only, with no contribution from Π_1^L , since this negative flux is associated with crossing from the right. However, $\Pi_{3,+}^L$ alone (which in the figure is indistinguishable from the total $\Pi_{3,+}$) provides incident and reflected bumps even though they are associated with different crossing directions. Recall in this respect that the superscript L in $\Pi_{3,+}^L$ means “motion from the left (positive momentum) *in the infinite past*”. (The reflected part will be seen in more detail in a different collision described in Fig. 5 below.) The difference $\Pi_1^L - \Pi_1^R$ has also been depicted; note its agreement with the flux.

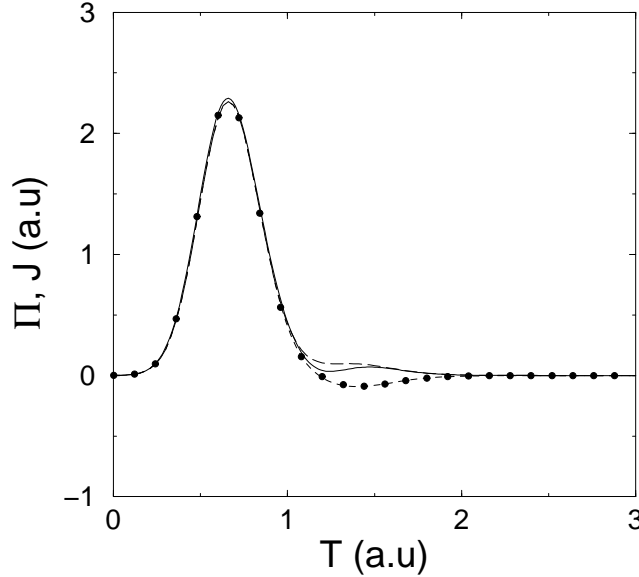


FIG. 3. J (dots), $\Pi_{3,+}$ (solid line), Π_1 (long dashed line), and $\Pi_1^L - \Pi_1^R$ (short dashed line) for $X = -2$.

At $X = 12$ there is only transmission and Π_1 , $\Pi_{3,+}$ and J are indistinguishable. However, for $X = 5$, i.e. in the barrier, $\Pi_{3,+}$ is clearly larger than J and Π_1 , which essentially coincide, see Fig. 4. A simple estimate of the ratio between the peaks follows from the classical limit discussed in the previous section: Π_1 must be to a good approximation proportional to an average local momentum; with the current parameters this entails $[2(18-10)]^{1/2} = 4$.

It is important to notice that the relevant quantity is the total energy (taken as ≈ 18 from the initial value of the momentum) *minus* the potential barrier energy. On the other hand, $\Pi_{3,+}$ is proportional to the square root of the total energy, $(2 \times 18)^{1/2} = 6$. The ratio of the two peaks in the figure is indeed 6:4.

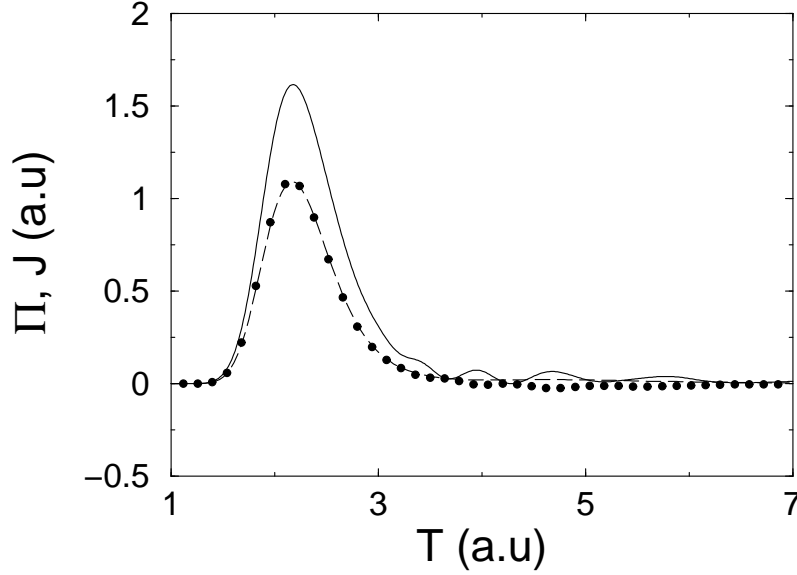


FIG. 4. J (dots), $\Pi_{3,+}$ (solid line), and Π_1 (dashed line) for $X = 5$.

As a complement to Figure 3, we have lowered the average momentum of the initial wave packet to $\langle \hat{p} \rangle = 3$, while keeping $\Delta x = 1$, so that the whole packet is now reflected. We evaluate J and all distributions at $x = -5$ for an initial average position $\langle \hat{x} \rangle = -9$. The flux, as portrayed in Fig. 5, shows clearly a positive part during the incidence and a negative part corresponding to reflection. Since several combinations of the different distributions and their components match with adequately the two bumps of $|J|$ or just one of those, we have in fact only represented $\Pi_{3,+} = \Pi_{3,+}^L$, with a dashed line. Π_1 is barely distinguishable from it. The incidence bump on the left is also reproduced by $\Pi_{2,+}$, or by Π_1^L , whereas the reflection bump is reproduced by $\Pi_{2,-}$ or Π_1^R .

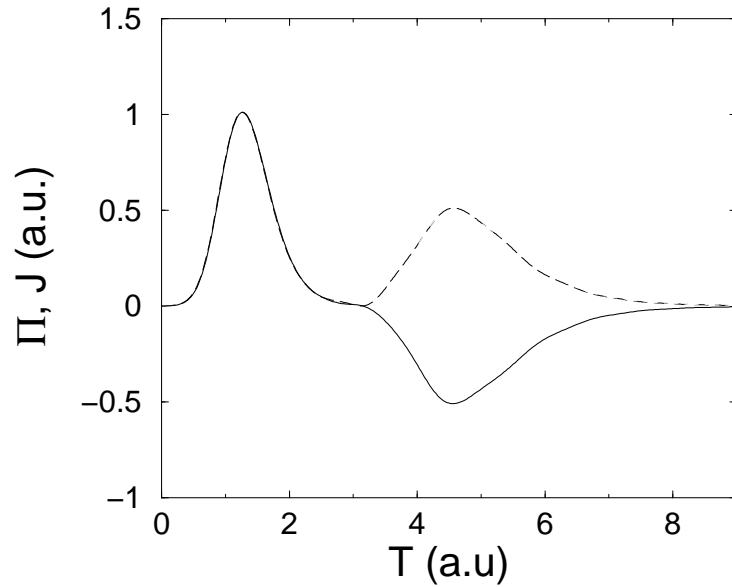


FIG. 5. J (solid line) and $\Pi_{3,+}$ (dashed line) for $X = -5$. See the text for details.

IV. CONCLUSION

We have examined three different generalizations for Kijowski's time-of-arrival distribution in the interacting case, both formally and numerically. This exam has yielded the result that, among these three, there is only one, Π_1 , in fact the simplest, that satisfies the correspondence principle in the sense of recovering the classical expression for the time of arrival when the effects of non-commutativity of the operators involved may be neglected. The other two proposals provide the correct classical limit in certain cases, but not in general. The numerical analysis of these distributions supports these formal considerations.

In order to make an adequate comparison between these three proposals, it has proved convenient to write them in the unified formalism of the "crossing states". The formalism itself suggests further generalizations, by considering alternative crossing states. An open question is whether the crossing state formalism is indeed the most adequate one for the description of times of arrival, or whether other presentations are more suitable. What is assured is both that the crossing state formalism guarantees covariance and positivity, and its power for comparing widely diverging previous proposals, this being a property that we would expect to hold more generally.

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